

Daresbury Laboratory INFORMATION QUARTERLY FOR COMPUTER SIMULATION OF CONDENSED PHASES

An informal Newsletter associated with Collaborative Computational Project No.5 on Molecular Dynamics, Monte Carlo & Lattice Simulations of Condensed Phases.

Number	39
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October 1993

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General News

This issue contains the abstracts of the talks given at the CCP5 annual meeting on "Large

- Scale Molecular Simulation" held at Keele. Also included are a number of short contribu-
- tions resulting from a workshop on calculating pressures held at Daresbury.
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STEERING COMMITTEE MEETING OF CCP5

A meeting of the steering committee of CCP5 was held on 15th. September 1993 at the University of Keele. Three new members of the executive committee were elected at this meeting. They are Prof. G. D. Price (Department of Earth Sciences, University College London), Dr. G. Jackson (Department of Chemistry, University of Sheffield), Dr. S. C. Parker (Department of Chemistry, University of Bath). The other members of the executive committee are Dr. M. Allen (Dept. of Physics, Bristol), Dr. J. Goodfellow (Dept. of Crystallography, Birkbeck College London) Dr. W. Mackrodt (ICI) and the chairman, Prof. M. Gillan (Department of Physics, University of Keele),

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A summary table is given below, further details may be found inside.

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TOPIC	DATES	LOCATION	
CCP5 Spring School on "Methods	11-15 April 1994	Southampton	
in Molecular Simulation"			
The development of improved in-	4-5 July 1994	Oxford	
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methods		a a sa ta sa ta sa sa	
The modelling of condensed phases	18-20 July 1994	Manchester	l ta da
using cellular automata	(Provisional)	ala segunda karala	

CCP5 PROGRAM LIBRARY of the state of the sta

Details are contained in this issue of accessing the CCP5 program library through E-mail automatically. Also details of accessing the Allen/Tildesley example programs at Cornell. New additions to the library from our readers are always welcome.

CRAY NEWS

CCP5 participants are reminded that CCP5 has an annual allocation of Cray time at Rutherford Laboratory. This is available for the development of simulation programs which are of general use to the CCP5 community. Readers who wish to use some of this allocation should write to the CCP5 Secretary, Dr. M. Leslie, TCS Division, SERC Daresbury Laboratory, Daresbury, Warrington WA4 4AD.

INTEL NEWS

CCP5 also has an annual allocation of time on the Intel IPSC/860 at Daresbury. If any CCP5 member wishes to make use of some of this time please contact M. Leslie at Daresbury.

CCP5 FUNDS FOR COLLABORATIONS

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CCP5 can make available funds of up to £200 per annum for groups of two or more UK researchers wishing to undertake a collaborative project within the scientific area covered by CCP5. The funds are intended to cover travel and subsistence costs. Researchers who wish to apply for funds are requested to submit a brief proposal (about 1/2 a page) describing the intended work to Dr. M. Leslie, SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire. Alternatively reply by Email to M.LESLIE@UK.AC.DARESBURY

CCP5 VISITORS PROGRAM

CCP5 organises a visitors program which funds the visit to the UK of overseas collaborators. We would normally expect a visitor to visit three sites in the UK and give a lecture at each site. These lectures would be open to all members of CCP5 as well as members of the host university. The visit would normally last between one or two weeks. CCP5 would pay for the cost of travel to the UK and within the UK between universities. CCP5 would expect some contribution towards accommodation expenses at the host university to be met by the university. We will also consider longer collaborations or visits just one place if this can be justified by the nature of the work to be done. If you have an overseas collaborator who you would like to invite under this program, please make a request to Dr. M. Leslie, SERC Daresbury Laboratory, Daresbury, Warrington, Cheshire. UK Alternatively reply by Email to M.LESLIE@UK.AC.DARESBURY

JANET:	M.LESLIE@DARESBURY					
INTERNET:	M.LESLIE@daresbury.ac.uk		n en en en Na en en en		 	
EARN/BITNET:	M.LESLIE%daresbury.ac.uk@ukacrl		::	· · · ·	 .:	. :

REQUEST FOR CONTRIBUTIONS

The deadline for contributions for the next 2 newsletters will be 15 December 1993 and 15 March 1994 Readers are reminded that contributions are always welcome. Contributions may be sent by Email in IAT_EX ; this makes the task of collating the newsletter simpler for the editor.

Contributors to the current issue

M. P. Allen	University of Bristol	n an an thair an thai
 D. Fincham W. Smith T. Forester	Keele University Daresbury Laboratory	a nazar nang si sa si na si si si si sa si sa si si na si si si sa si sa si si si na si si sa si si si si si si na si si si sa si
A. J. Masters	Manchester University	a a si da ⁿ asa
D. M. Heyes	University of Surrey	and the state of the second

CCP5 SPRING SCHOOL ON

METHODS IN MOLECULAR SIMULATION

SERC's collaborative computational project number 5 (CCP5) is organising a school for graduate students on "Methods in Molecular Simulation". This residential school will take place from Monday 11 April 1994 to Friday 15 April at the University of Southampton. The school will be limited to 30 students and preference will be given to first- and secondyear graduate students from the U.K. working in the area of molecular simulation.

A provisional programme for the school consists of the following lectures:

1.	the basic Monte Carlo method;
2.	biased sampling techniques in Monte Carlo simulations, and the second state
3.	Monte Carlo simulations of chain molecules and polymers;
4.	basic molecular dynamics;
5.	molecular dynamics in various ensembles;
6.	constraint dynamics;
7.	equilibrium properties and structure;
8.	time correlation functions and spectra;
9.	nonequilibrium simulations;
10.	long-range forces; provide the state of the
11.	free energy calculations;
12.	Gibbs ensemble simulations;

13. Simulation on parallel computers.

The lectures will be supported by a full programme of practical workshops which will enable the graduate students to use the Silicon Graphics Indigo workstations in the University of Southampton's data visualisation facility. There will be an invited seminar each evening to allow students to hear some of the most recent developments in molecular simulation.

The school will be organised by Mike Allen (Bristol) and Dominic Tildesley (Southampton). The cost for the school will be £140 for the week. This includes bed, breakfast, dinner, photocopied course notes and other supplementary material. Please send applications on the attached form to

Professor D.J. Tildesley Department of Chemistry The University of Southampton Southampton S09 5NH. Applications will be considered in order of their receipt. In the event that the Course is over-subscribed, 1st year students will be given preference over 2nd year students. It is possible to apply to the SERC for support to send students to this meeting and details will be sent to supervisors on receipt of the applications.

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POSTDOCTORAL POSITION Computer simulation of liquid crystals

A postdoctoral position will be available starting October 1 1993 (or shortly thereafter) for up to three years, working in the area of computer simulation of liquid crystals using idealized models. The post is funded by SERC, and the principal objectives are: (i) the computer simulation of twisted and chiral liquid crystal phases and measurement of their properties; (ii) precise location and characterization of phase transitions involving mesophases; (iii) simulation of liquid crystalline polymers. The group uses a network of Unix workstations, a massively-parallel computer, and time on local and national supercomputers; the grant for this project includes funding for a substantial enhancement of the local computer power. This position would be suitable for someone with experience in simulating statistical mechanical systems, preferably in the complex fluids area, and the starting salary is $\sim \pounds 15k/year$.

	Dr. M. P. Allen	
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	email: M.P.Allen@bristol.ac.uk	
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CCP5 Program Library Conditions of Distribution

The CCP5 Program Library provides programs and documentation free of charge to academic centres upon application to Dr. W. Smith, TCS Division, S.E.R.C. Daresbury Laboratory, Daresbury, Warrington WA4 4AD, U.K. Please supply a magnetic tape to receive the copies. Industrial and commercial applicants should enclose a £100 handling charge. No magnetic tape need be sent in this case. Listings of programs are available if required. Please note that use of inappropriate packing for magnetic tapes (e.g. padded bags) may result in them being returned without the required software. Please ensure that these forms of packaging are not used. A list of programs available is presented in the following pages.

All applicants will be required to sign an agreement not to exploit the programs for commercial purposes e.g. for resale or distribution as part or whole of a commercial product.

Readers should also note that we are authorised to supply the example programs originally published in the book "Computer Simulation of Liquids", by M.P. Allen and D.J. Tildesley (Clarendon Press, Oxford 1987). These are supplied in the same manner as the resident CCP5 programs. We are grateful to Mike Allen and Dominic Tildesley for their permission.

We should also like to remind our readers that we would welcome further contributions to the Program Library. The Library exists to provide support for the research efforts of everyone active in computer simulation and to this end we are always pleased to extend the range of software available. If any of our readers have any programs they would like to make available, please would they contact Dr. Smith.

Please Note: For copyright reasons we are not able to supply the programs CASCADE, SYMLAT, THBFIT, THBPHON and THBREL free of charge to Universities outside the United Kingdom.

Programs from the Book: "Computer Simulation of Liquids" by M.P. Allen and D. Tildesley, Clarendon Press, Oxford 1987.

These programs originally appeared on microfiche in the book "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley, published by Oxford University Press, 1987. They are made freely available to members of CCP5, in the hope that they will be useful. The intention is to clarify points made in the text, rather than to provide a piece of code suitable for direct use in a research application. We ascribe no commercial value to the programs themselves. Although a few complete programs are provided, our aim has been to offer building blocks rather than black boxes. As far as we are aware, the programs work correctly, but we can accept no responsibility for the consequences of any errors, and would be grateful to hear from you if you find any. You should always check out a routine for your particular application. The programs contain some explanatory comments, and are written, in the main, in FORTRAN-77. One or two routines are written in BASIC, for use on microcomputers. In the absence of any universally agreed standard for BASIC, we have chosen a very rudimentary dialect. These programs have been run on an Acorn model B computer. Hopefully the translation of these programs into more sophisticated languages such as PASCAL or C should not be difficult.

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CCP5 Program Library E-Mail Service

From January 1 1991 it will be possible for CCP5 members to get copies of CCP5 programs through E-mail *automatically*. To do so they should send an E-mail message to **info-server@uk.ac.daresbury**. The contents of the e-mail message should be as follows (Note: the use of upper and lower case is significant - this is a unix system!):

request sources to be a series of the series

Where program-name is the name of the desired source code. A mail server will automatically process this message and return a copy of the source code to your e-mail address. Please note the following however:

The program source will be returned to you in uue format, which is a form of encoding most suitable for mail messages. It can easily be decoded on any unix system using the uudecode command. (Check your local unix man file for details). Also, to speed the transfer, the source will be split into files of 1200 records each, so expect two or three such files for the average CCP5 program. Once again, uudecode will help you to sort things out.

Readers who do not have unix facilities should include the following lines at the start of the above message:

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line-limit: nnnnn; state state of A Association for the state state state state of the state of the coding: off

Where nnnnn is the number of records in the source (in most cases 6000 should be enough). The program will be sent in plain FORTRAN as a single file. It may take a while to arrive, but be patient! Also beware in case your system mailer cannot handle messages of this size.

The programs from "Computer Simulation of Liquids" are also available. To access them use program-name F.01, for example.

Readers must realise that the terms of use and distrubution of the CCP5 programs that have applied hitherto will be maintained. Users should not redistribute or sell the programs, nor is any liability accepted for their use, either by SERC or the program authors. It is a requirement on the user that the programs be fully tested for their intended purpose. Any bugs found should be reported to the librarian, for the benefit of other users.

Lastly readers should realise that this means of transfer does not include any program

documentation. So if you are unable to make sense of the programs, write for the documentation! We are grateful to Mr. P. Griffiths of Daresbury's ITS Division for implementing this facility.

Availability of the Allen/Tildesley example programs at Cornell

Appendix F of the Book "Computer Simulation of Liquids" by M. P. Allen and D. J. Tildesley describes a method whereby the example programs may be obtained from the statistical mechanics group FTP facility at Cornell. This facility is no longer operational as advertised, due to software and hardware changes. However, the programs are still available. To obtain them, please follow the procedure outlined here. The description below is taken from the HELP file that is distributed by the file server; to obtain the Allen/Tildesley example programs, simply use "ALLEN_TILDESLEY" as the package name (without the quotes, note underscore character _ not hyphen -).

STATMECH is a file distribution service for the Statistical Mechanics community that uses electronic mail facilities to deliver files. To communicate with STATMECH, send an EMAIL message to: statmech@cheme.tn.cornell.edu Commands are sent in the body of hte message you send to STATMECH (not in the subject line). Several commands may be sent at one time; just put one command per line.

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SENDME package	Sends all parts of the specified package.
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For each request you make, a transaction log is returned to you indicating the status of the request. The status report will indicate whether the request was successfully completed, and when the file was or will be sent. Large files are sent only during offpeak hours.

Problems, questions and comments about STATMECH service on this system should be directed to "statmech-mgr@cheme tn.cornell.edu".

Steve Thompson, School of Chemical Engineering, Cornell University, Ithaca NY 14853 USA.

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THE CCP5 PROGRAM LIBRARY.

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SCN	[MC,LJA,	RFD,TH]	N. Corbin		
SMFK [MC-SCF, Cylindrical Polyelec.] A.P. Lyubartsev					
SLS_PRO [MD, Proteins, LF, TH+RDF] A. Raine					
SOTON_PAR	[MD,LJA,	LC,TH] M	I.R.S. Pinches		
SURF	[MD,BEM/	TF/2D,LF	,TH+RDF] D.M. Heyes	n na sa ti	
SYMLAT [LS,PIL,EM+SYM,TH+STR] Barwell					
TEQUILA [GP] A. Wilton and F. Mueller-Plathe					
THBFIT	[LS,PIL,	EM,Poter	tial fitting] Harvell		
THEPHON	[LS,PIL/	38,EM,Ph	nonon dispersion] Harwell		
THBREL	[LS,PIL,	EM, TH+ST	[R] Harwell		
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Program types:		MD	Molecular dynamics	141144	
		MC	Monte Carlo		
		PRMD	Parrinello-Rahman MD		
		LS	Lattice simulations		
		SD	Stochastic dynamics	14.311	
		DA	Data analysis	ana ana i	
		UT	Utility package		
		PIMC	Path Integral Monte Carlo		
		GP	Graphics program		
		5. S. J.	a de la companya de La companya de la comp		
System mod	lels:	LJA	Lennard-Jones atoms		
		LJD	Lennard-Jones diatomic molecules		
		LJL	Lennard-Jones linear molecules		
		LJT	Lennard-Jones tetrahedral molecules		
		LJS	Lennard-Jones site molecules		
		RPE	Restricted primitive electrolyte	10.043	
		BHM	Born-Huggins-Meyer ionics	a de tra	
		SGWP	Spherical gaussian wavepackets		
		TF	Tosi-Fumi ionics		
		VS	Variable site-site model	- 1 A. A. 10	
		BA	Bond angle model	E Creek	
		PD	Point dipole model		
		PQ	Point quadrupole model		
		MIX	Mixtures of molecules		
		GAU	Gaussian molecule model	a poper d	
		FC.	Fractional charge model		
		PIL	Perfect ionic lattice model		
		DIL	Defective ionic lattice model		
		3B	3-body force model		
		2D	Two dimensional simulation		
		SF	Shifted force potential	1.1.1	
		FC	Fractional charge model		
	• •	AQ	Aqueous solutions		

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Algorithm: G5 Gear 5th order predictor-corrector Q4 Quaternion plus 4th. order Gear P-C. LF Leapfrog (Verlet) 0F Fincham Quaternion algorithm 05 Sonnenschein Quaternion algorithm Link-cells MD algorithm LC CP Constant pressure CT Constant temperature ΤA Toxvaerd MD algorithm CA Constraint algorithm EM Energy minimisation Symmetry adapted algorithm SYM Rossky-Friedman-Doll algorithm RFD Thermostatted SLLOD equations SLLOD a sector de la construcción de la c Thermodynamic properties. TH Properties: Mean-square-displacement Radial distribution function Structure factor MSD RDF STF energia energia. Velocity autocorrelation function VACF Quantum corrections QC. Lattice stresses STR and the second second states we are a second s

Programs from the Book "Computer Simulation of Liquids"

Periodic boundary conditions in various geometries F.1 F.2 5-value Gear predictor-corrector algorithm F.3 Low-storage MD programs using leapfrog Verlet algorithm Velocity version of Verlet algorithm F.4 F.5 Quaternion parameter predictor-corrector algorithm Leapfrog algorithms for rotational motion F.6 F.7 Constraint dynamics for a nonlinear triatomic molecule Shake algorithm for constraint dynamics of a chain molecule F.8 Rattle algorithm for constraint dynamics of a chain molecule F.9 F.10 Hard sphere molecular dynamics program F.11 Constant-NVT Monte Carlo for Lennard-Jones atoms F.12 Constant-NPT Monte Carlo algorithm F.13 The heart of a constant \$\mu\$VT Monte Carlo program Algorithm to handle indices in constant \$\mu\$VT Monte Carlo F.14 Routines to randomly rotate molecules F.15 F.16 Hard dumb-bell Monte Carlo program F.17 A simple Lennard-Jones force routine Algorithm for avoiding the square root operation F.18 F.19 The Verlet neighbour list F.20 Routines to construct and use cell linked-list method F.21 Multiple timestep molecular dynamics F.22 Routines to perform the Ewald sum F.23 Routine to set up alpha fcc lattice of linear molecules F.24 Initial velocity distribution F.25 Routine to calculate translational order parameter F.26 Routines to fold/unfold trajectories in periodic boundaries F.27 Program to compute time correlation functions F.28 Constant-NVT molecular dynamics - extended system method F.29 Constant-NVT molecular dynamics - constraint method F.30 Constant-NPH molecular dynamics - extended system method F.31 Constant-NPT molecular dynamics - constraint method F.32 Cell linked-lists in sheared boundaries F.33 Brownian dynamics for a Lennard-Jones fluid F.34 An efficient clustering routine F.35 The Voronoi construction in 2d and 3d F.36 Monte Carlo simulation of hard lines in 2d F.37 Routines to calculate Fourier transforms

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Calculating the Pressure

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1 Basics

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In standard thermodynamics the pressure \mathcal{P} is given by the relation

$$\mathcal{P} = -\left(\frac{\partial A}{\partial V}\right)_T \tag{1}$$

where A is the Helmholz free energy, V the volume and T the temperature. This can be expanded into

$$\mathcal{P} = \frac{1}{\beta} \left(\frac{\partial}{\partial V} \log Q_N(V, T) \right)_T$$
(2)

or

$$\mathcal{P} = \frac{1}{\beta Q_N(V,T)} \left(\frac{\partial}{\partial V} Q_N(V,T) \right)_T$$
(3)

where $Q_N(V,T)$ is the partition function

$$Q_N = \frac{1}{N! \ h^{3N}} \int \int \exp(-\beta H_N(\underline{r}^N, \underline{p}^N)) \ d\underline{r}^N d\underline{p}^N \tag{4}$$

and $H_N(\underline{r}^N, \underline{p}^N)$ is the system Hamiltonian (assuming a canonical ensemble).

In order to calculate the pressure from these expressions it is necessary to introduce the scaling relations:

$$\underline{r}_i = V^{1/3} \underline{s}_i, \qquad \underline{\pi}_i = V^{2/3} m_i \underline{s}_i, \qquad \underline{p}_i = V^{-1/3} \underline{\pi}_i, \qquad (5)$$

where $\{\underline{r}_i, \underline{p}_i\}$ and $\{\underline{s}_i, \underline{\pi}_i\}$ are conjugate pairs of atomic positions and momenta in real and 'scaled' space respectively. Use of these relations allows the pressure equation to be written as

$$\mathcal{P} = -\frac{1}{(N!h^{3N}Q_N(V,T))} \int \int \left(\frac{\partial}{\partial V} H_N(V^{1/3}\underline{s}^N, V^{-1/3}\underline{\pi}^N)\right)_T \times \exp(-\beta H_N(V^{1/3}\underline{s}^N, V^{-1/3}\underline{\pi}^N)) \, d\underline{s}^N d\underline{\pi}^N \tag{6}$$

or in other words

$$\mathcal{P} = -\left\langle \left(\frac{\partial}{\partial V} H_N(V^{1/3} \underline{s}^N, V^{-1/3} \underline{\pi}^N) \right)_T \right\rangle$$
(7)

which is the fundamental equation of the method.

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2 Example Applications

2.1 Simple Atomic System with Pair forces

The Hamiltonian for such a system is the transformer and the second states and the second states and the second

$$H_N(\underline{r}^N, \underline{p}^N) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i=2}^N \sum_{j < i} U(r_{ij}),$$
(8)

where r_{ij} is the separation between atoms i and j. This may be transformed using the scaled variables into

$$H_N(V^{1/3}\underline{s}^N, V^{-1/3}\underline{\pi}^N) = V^{-2/3} \sum_{i=1}^N \frac{\pi_i^2}{2m_i} + \sum_{i=2}^N \sum_{j < i} U(V^{1/3}s_{ij})$$
(9)

It is easy to show that

$$\frac{\partial H_N}{\partial V} = -\frac{2}{3V} V^{-2/3} \sum_{i=1}^N \frac{\pi_i^2}{2m_i} + \frac{1}{3V} V^{1/3} \sum_{i=2}^N \sum_{j < i} U'(V^{1/3} s_{ij}) s_{ij}, \tag{10}$$

where U'(x) is the first derivative of U(x) with respect to the argument x. This relation can be transformed back into the original variables as

$$\frac{\partial H_N}{\partial V} = -\frac{2}{3V} \sum_{i=1}^N \frac{p_i^2}{2m_i} + \frac{1}{3V} \sum_{i=2}^N \sum_{j < i} \frac{1}{r_{ij}} U'(r_{ij}) \underline{r}_{ij} \cdot \underline{r}_{ij}$$
(11)

where the scalar product $\underline{r}_{ij} \cdot \underline{r}_{ij}$ has been introduced into the second rhs term to bring out the relationship between this term and the usual virial.

The pressure in this system is therefore:

$$\mathcal{P} = \frac{1}{3V} \left\langle 2 \sum_{i=1}^{N} \frac{p_i^2}{2m_i} - \sum_{i=2}^{N} \sum_{j < i} \frac{1}{r_{ij}} U'(r_{ij}) \underline{r}_{ij} \cdot \underline{r}_{ij} \right\rangle$$
(12)

which is the same as the form given by the virial theorem.

2.2 Flexible Polyatomic Molecules death which careade be reached and the

The Hamiltonian for a system of flexible polyatomic molecules (i.e. without constrained bonds and angles *etc*) is commonly of the form:

$$H_N(\underline{r}^N, \underline{p}^N) = \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i=2}^N \sum_{j < i} U^{nb}(r_{ij}) + \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i=2}^N \sum_{j < i} U^{nb}(r_{ij}) + \sum_{i=1}^N \frac{p_i^2}{2m_i} + \sum_{i=2}^N \frac{p_i^2}{2m_i} + \sum_{i$$

$$\sum_{k=1}^{N_b} U_k^b(r_{ab}) + \sum_{k=1}^{N_t} U_k^t(\underline{r}_a, \underline{r}_b, \underline{r}_c) +$$
(13)

$$\sum_{k=1}^{N_f} U_k^f(\underline{r}_a, \underline{r}_b, \underline{r}_c, \underline{r}_d)$$
 and the second se

Clearly, the kinetic energy, nonborded terms (U^{nb}) and bonded terms U_k^b may be treated in exactly the same way as the previous case. The three body (U_k^t) and four body terms need to be considered on a case-by-case basis.

In dealing with three body terms, three common cases occur:

- 1. $U_k^t(r_{ab}, r_{bc}, r_{ac})$; the potential depends on three spatial separation between three atoms (e.g. Axilrod-Teller potential). This becomes $U_k^t(V^{1/3}s_{ab}, V^{1/3}s_{bc}, V^{1/3}s_{ac})$ after the scaling transformation, which on differentiation wrt V clearly contributes to the virial.
- 2. $U_k^t(\hat{r}_{ab}, \hat{r}_{bc})$; the potential depends on the relative positions of three atoms, but it is the angles between the vectors that determine the potential (e.g. the valence angle potential). These potentials are unaffected by the scaling transformation and so cannot contribute to the pressure.
- 3. $U_k^t(\hat{r}_{ab}, \hat{r}_{bc}) \times S(r_{ab}, r_{bc})$; the potential has both an angular part and a 'switching' function which zeroes the potential at long range (e.g. the Leslie three body potential). Provided the switching function is analytical, the scaling transformation gives $U_k^t(\hat{r}_{ab}, \hat{r}_{bc}) \times S(V^{1/3}s_{ab}, V^{1/3}s_{bc})$, which clearly will contribute to the pressure.

With regard to four body terms, the only common potential (that I am aware of) is the dihedral angle potential: $U_k^f(\hat{r}_{ab}, \hat{r}_{bc}, \hat{r}_{cd})$; which has no dependence on interatomic distance, and hence no contribution to the pressure.

2.3 Diatomic Molecule with Extensible Bond backweyeek advances and

The atomic positions of the i'th molecule are given by because we make developments and

$$\underline{R}_i^a = \underline{R}_i + \underline{d}_i^a \qquad \underline{R}_i^b = \underline{R}_i + \underline{d}_i^b$$
(14)

with

$$\underline{d}_{i}^{a} = -\frac{\mu_{i}}{m_{i}^{a}}\underline{B}_{i} \qquad \underline{d}_{i}^{b} = \frac{\mu_{i}}{m_{i}^{b}}\underline{B}_{i}$$
(15)

Where \underline{R}_i locates the molecule COM and \underline{B}_i is the bond vector. Vectors \underline{d}_i^a and \underline{d}_i^b define the positions of atoms a abd b respectively, wrt the centre of mass. m_i^a and m_i^b are atomic masses μ_i the reduced mass. (The molecule mass will be designated M_i .)

The partition function is

$$Q_N(V,T) = \mathcal{N} \int \dots \int \exp(-\beta H_N(\underline{R}^N, \underline{B}^N, \underline{P}^N, \underline{Q}^N)) \, d\underline{R}^N d\underline{B}^N d\underline{P}^N d\underline{Q}^N, \quad (16)$$

The appropriate scaled (conjugate) coordinates are

$$\underline{R}_{i} = V^{1/3} \underline{S}_{i} \qquad \underline{\Pi}_{i} = V^{2/3} M_{i} \underline{S}_{i} \qquad \underline{P}_{i} = V^{-1/3} \underline{\Pi}_{i}$$
(17)

$$\underline{B}_{i} = V^{1/3} \underline{D}_{i} = V^{1/3} \underline{D}_{i} + V^{2/3} \underline{\mu}_{i} = V^{2/3} \mu_{i} \underline{D}_{i} + \cdots + \underline{Q}_{i} = V^{-1/3} \underline{\Lambda}_{i} + \cdots + (18)$$

The pressure is therefore

$$\mathcal{P} = -\left\langle \left(\frac{\partial}{\partial V} H_N(V^{1/3} \underline{S}^N, V^{1/3} \underline{D}^N, V^{-1/3} \underline{\Pi}^N, V^{-1/3} \underline{\Lambda}^N) \right)_T \right\rangle$$
(19)

where, assuming atom-atom pair forces, the Hamiltonian is

$$H_N(V^{1/3}\underline{S}^N, V^{1/3}\underline{D}^N, V^{-1/3}\underline{\Pi}^N, V^{-1/3}\underline{\Lambda}^N) =$$
(20)

$$V^{-2/3} \sum_{i=1}^{N} \frac{\Pi_i^2}{2M_i} + V^{-2/3} \sum_{i=1}^{N} \frac{\Lambda_i^2}{2\mu_i} + \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{2} \sum_{b=1}^{2} U^{ab} (V^{1/3} S_{ij}^{ab}) + \sum_{i=1}^{N} U^b (V^{1/3} D_i)$$
(21)

with

$$\underline{S}_{ij}^{ab} = V^{-1/3} \underline{R}_{ij}^{ab} = V^{-1/3} \left(\underline{R}_j - \underline{R}_i + \underline{d}_j^b - \underline{d}_i^a \right)$$
(22)

With these formulae it can be shown that

$$\mathcal{P} = \frac{2}{3V} \left\langle \left(V^{-2/3} \sum_{i=1}^{N} \frac{\Pi_i^2}{2M_i} + V^{-2/3} \sum_{i=1}^{N} \frac{\Lambda_i^2}{2\mu_i} \right) \right\rangle - \frac{1}{3V} \left\langle \left(\sum_{i=2}^{N} \sum_{j < i} V^{1/3} \sum_{a=1}^{2} \sum_{b=1}^{2} U'^{ab}(R_{ij}^{ab}) S_{ij}^{ab} + V^{1/3} \sum_{i=1}^{N} U'^{b}(B_i) D_i \right) \right\rangle$$
(23)

which is easily reduced to some standard and a second decaded to an application and the

$$\mathcal{P} = \frac{1}{3V} \left\langle 2\sum_{i}^{N} \left(\frac{P_i^2}{2M_i} + \frac{Q_i^2}{2\mu_i} \right) + \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{2} \sum_{b=1}^{2} \underline{f}_{ij}^{ab} \cdot \underline{R}_{ij}^{ab} + \sum_{i=1}^{N} \underline{f}_{ii}^{ab} \cdot \underline{B}_i \right\rangle$$
(24)

Comments

1. Note that the expression for the pressure includes the rotational kinetic energy.

2.4 Rigid Diatomic Molecules

The partition function is

$$Q_N(V,T) = \mathcal{N} \int \dots \int \exp(-\beta H_N(\underline{R}^N, \Omega^N, \underline{P}^N, \Lambda^N)) \, d\underline{R}^N d\Omega^N d\underline{P}^N d\Lambda^N, \qquad (25)$$

where $\Omega^N = (\Theta^N, \Phi^N)$ are the angles defining the molecular orientations and $\Lambda^N = (\Lambda^N_\theta, \Lambda^N_\phi)$ their respective conjugate momenta. The momenta are given by

$$\underline{P}_{i} = M_{i}\underline{R}_{i}, \qquad \Lambda_{i\theta} = \mu_{i}B_{i}^{2}\dot{\Theta}_{i}, \qquad \Lambda_{i\Phi} = \mu_{i}B_{i}^{2}\cos^{2}(\Theta)_{i}\dot{\Phi}_{i}.$$
(26)

 B_i is the (constant) bondlength of molecule *i*, so as set as set of a sympletic value of Using the scaling relation and its conjugate momentum:

$$\underline{R}_{i} = V^{1/3} \underline{S}_{i} \qquad \underline{\Pi}_{i} = V^{2/3} M_{i} \underline{S}_{i} \qquad \underline{P}_{i} = V^{-1/3} \underline{\Pi}_{i}, \text{ for a set of a set of }$$
(27)

the pressure can be written directly as

$$\mathcal{P} = -\left\langle \left(\frac{\partial}{\partial V} H_N(V^{1/3} \underline{S}^N, \Omega^N, V^{-1/3} \underline{\Pi}^N, \Lambda^N) \right)_T \right\rangle^2, \qquad (28)$$

It is obvious that there can be no scaling of the angular coordinates. Assuming all the forces arise from atom-atom interactions and using the relations

$$\underline{R}_{i}^{a} = \underline{R}_{i} + \underline{d}_{i}^{a} \qquad \underline{R}_{i}^{b} = \underline{R}_{i} + \underline{d}_{i}^{b}$$
⁽²⁹⁾

with

$$\underline{d}_{i}^{a} = -\frac{\mu_{i}}{m_{i}^{a}}\underline{B}_{i} \qquad \underline{d}_{i}^{b} = \frac{\mu_{i}}{m_{i}^{b}}\underline{B}_{i}$$
(30)

as before, we note that the scaling affects only the centre of mass coordinates:

$$\underline{R}_{ij}^{ab} = V^{1/3} \underline{S}_{ij} + \underline{d}_j^b - \underline{d}_i^a$$
(31)

where $V^{1/3}\underline{S}_{ij} = \underline{R}_{ij}$ is the distance between molecules *i* and *j* (wrt COM). We can write

$$\mathcal{P} = \frac{1}{3V} \left\langle 2\sum_{i=1}^{N} \frac{P_i^2}{2M_i} - \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{2} \sum_{b=1}^{2} \frac{1}{R_{ij}^{ab}} U'^{ab}(R_{ij}^{ab}) \underline{R}_{ij}^{ab} \cdot \underline{R}_{ij} \right\rangle$$
(32)

; From equation (31) this may be rewritten as

$$\mathcal{P} = \frac{1}{3V} \left\langle 2\sum_{i=1}^{N} \frac{P_i^2}{2M_i} + \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{2} \sum_{b=1}^{2} \underline{f}_{ij}^{ab} \cdot \underline{R}_{ij}^{ab} - \sum_{i=1}^{N} \sum_{a=1}^{2} \underline{f}_i^a \cdot \underline{d}_i^a \right\rangle$$
(33)
the force on atom *a* of molecule *i*.

where \underline{f}_{i}^{a} is the force on atom a of molecule *i*.

Comments

- 1. There is now no term corresponding to the rotational kinetic energy in the pressure.
- 2. The last term rhs is a manifestation of the constraint force, which appears as an additional term acting on the atoms to keep them bonded. However is not the complete constraint force, which also includes contributions from centripetal
- forces.
- 3. The absence of centripetal forces is the reason the rotational kinetic energy term is missing.
- 4. The appearance of the partial constraint force term implies that it is generally necessary to include the constraint forces in calculating the pressure. If the kinetic energy is evaluated atomistically, it will automatically include the necessary rotational energy.

2.5 Rigid Polyatomic Molecules

The partition function is

$$Q_N(V,T) = \mathcal{N} \int \dots \int \exp(-\beta H_N(\underline{R}^N, \Omega^N, \underline{P}^N, \Lambda^N)) d\underline{R}^N d\Omega^N d\underline{P}^N d\Lambda^N, \qquad (34)$$

where $\Omega^N = (\Theta^N, \Phi^N, \Psi^N)$ are the Euler angles defining the molecular orientations and $\Lambda^N = (\Lambda^N_{\theta}, \Lambda^N_{\phi}, \Lambda^N_{\psi})$ their respective conjugate momenta.

The scaling relation applies to the position vector and translational momentum;

$$\underline{R}_{i} = V^{1/3} \underline{S}_{i} \qquad \underline{\Pi}_{i} = V^{2/3} M_{i} \underline{S}_{i} \qquad \underline{P}_{i} = V^{-1/3} \underline{\Pi}_{i}.$$
(35)

The pressure is given by

$$\mathcal{P} = -\left\langle \left(\frac{\partial}{\partial V} H_N(V^{1/3} \underline{S}^N, \Omega^N, V^{-1/3} \underline{\Pi}^N, \Lambda^N) \right)_T \right\rangle, \tag{36}$$

where assuming all the forces arise from atom-atom pair interactions, the Hamiltonian is

$$H_N(V^{1/3}\underline{S}^N, \Omega^N, V^{-1/3}\underline{\Pi}^N, \Lambda^N) =$$
(37)

$$V^{-2/3} \sum_{i=1}^{N} \frac{\Pi_{i}^{2}}{2M_{i}} + \frac{1}{2} \sum_{i=1}^{N} \underline{\omega}_{i} \cdot \underline{I}_{i} \cdot \underline{\omega}_{i} + \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{n_{j}} \sum_{b=1}^{n_{j}} U(R_{ij}^{ab}).$$
(38)

In this equation, \underline{R}_{ij}^{ab} represents the separation vector between atoms a and b on molecules i and j respectively. i.e.

$$\underline{R}_i^a = \underline{R}_i + \underline{d}_i^a \tag{39}$$

with \underline{R}_i being the centre of mass and \underline{d}_i^a being the atomic displacement from the COM. Hence

$$\underline{R}_{ij}^{ab} = \underline{R}_{ij} + \underline{d}_{ij}^{ab} \tag{40}$$

and we note that $\underline{S}_{ij} = V^{-1/3} \underline{R}_{ij}$ is the scaled distance between molecules *i* and *j* (wrt COM). The pressure is therefore $\mathcal{P} = \frac{1}{3V} \left\langle 2 \sum_{i=1}^{N} \frac{P_i^2}{2M_i} - \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{n} \sum_{b=1}^{n} \frac{1}{R_{ij}^{ab}} U^{inb}(R_{ij}^{ab}) \underline{R}_{ij}^{ab} \cdot \underline{R}_{ij} \right\rangle$ (41)

which may be written as

$$\mathcal{P} = \frac{1}{3V} \left\langle 2\sum_{i=1}^{N} \frac{P_i^2}{2M_i} + \sum_{i=2}^{N} \sum_{j < i} \sum_{a=1}^{n_i} \sum_{b=1}^{n_i} \frac{f_i^{ab}}{f_{ij}} \cdot \underline{R}_{ij}^{ab} - \sum_{i=1}^{N} \sum_{a=1}^{n_i} \frac{f_i^a}{f_i} \cdot \underline{d}_i^a \right\rangle$$
(42)

where f_i^a is the force on atom *a* of molecule *i*.

References
[1] W. Smith, CCP5 Info. Quart. 26 43 (1987).

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Surface Stress of Point Charge Lattices

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In surface science it is quite a common problem to want to know the electrostatic potential near the surface of a crystal or ionic liquid. From a modelling point of view, the surface is usually represented by a two-dimensionally repeating unit cell of charges. The 2D vector, \underline{n} , denoting the position of the unit cell is given by,

$$\underline{n} = i\hat{x}L_{x} + j\hat{y}L_{y}, \qquad (1)$$

where the unit vectors $\hat{\gamma}$ are along the γ direction, the corresponding cell sidelengths are, L_{γ} and the integers i, j range over $0, \pm 1, \pm 2, \dots, \pm \infty$. The x and y directions form the surface plane. The z direction is perpendicular to the surface plane. Consider N point charges of index i with point charge values, q_i in a unit cell of volume, V. These charges are positioned at r_{ni} where $1 \leq i \leq N$ and \underline{n} indicates the lattice cell in which it is found. A semi-infinite or 'half-space' is built up from a series of these laminae positioned parallel and packed together.

The total coulomb interaction energy, Φ of the point charge system is,

$$2\Phi = \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{\underline{n}} q_i q_j r_{\underline{n}ij}^{-1}, \qquad (2)$$

where $r_{\underline{n}ij} = |\underline{r}_{\underline{n}ij}| = |\underline{r}_{\underline{n}i} - \underline{r}_{\underline{n}j}|$. There is a null entry in equation ?? for i = j when $\underline{n} = 0$.

For a bulk point charge lattice, Ewald recast this summation as two series, one in real space and the other in Fourier space (covering the reciprocal lattice). Both of these series can be caused to converge rapidly by a suitable choice of an arbitrary parameter, κ , present in both series. An analoguous procedure was followed by Parry [?] [?] for laminar and semi-infinite geometries. We have,

$$2\Phi = \frac{\sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{\underline{n}}^{\infty} q_i q_j er fc(\kappa r_{\underline{n}ij})}{r_{\underline{n}ij}} + \frac{\pi}{A} \sum_{\underline{h}}^{\infty} \sum_{i=1}^{N} q_i \sum_{j=1}^{N} q_j F(\kappa, \underline{h}, r_{zij}) \Re[\exp(i\underline{h}, \underline{r}_{ij})] - \sum_{i=1}^{N} \frac{2\kappa q_i^2}{\pi^{1/2}}, \qquad (3)$$

where $erfc(\cdots)$ is the complementary error function, r_{zij} is the z or 'out-of-plane' component of r_{nij} (the same for all <u>n</u>) and \Re denotes the real part of the complex quantity. The original summation of equation ?? is carried out in real space; however, in equation ?? this is transformed into two summations, one in real space (over the same real space lattice, <u>n</u>) and one in reciprocal space (over the reciprocal lattice, <u>h</u>). The quantity, κ is an adjustable parameter with units of inverse length. The value of κ determines the relative emphasis given to the real and reciprocal space terms; the reciprocal space series increasingly dominates in contribution as κ increases. The in-plane area of the unit cell, A, equals, $A = |\underline{L}_x \times \underline{L}_y|$. The reciprocal lattice vector is defined by,

$$\underline{h} = 2\pi (i\hat{x}/L_x + j\hat{y}/L_y). \tag{4}$$

Also,

$$F'(\kappa, \underline{h}, r_{zij}) = (\exp(hr_{zij})erfc(h/2\kappa + r_{zij}\kappa) + \exp(-hr_{zij})erfc(h/2\kappa - r_{zij}\kappa))h^{-1}, \quad (5)$$

for $h \neq 0$ and

$$F(\kappa, \underline{h} = 0, r_{zij}) = -2[r_{zij}erf(r_{zij}\kappa) + \exp(-(r_{zij}\kappa)^2)/\kappa\pi^{1/2}],$$
(6)

for h = 0.

The purpose of the talk was to show how the Parry formulae could be developed further to obtain the components of the stress tensor [?]. For example, the coulombic component of the stress tensor (including both real and reciprocal space series) for the xx, xy, yx and yy components is given by,

$$-S_{\alpha\beta}V = \sum_{i=1}^{N} q_i \sum_{j=1}^{N} q_j \sum_{\underline{n}}^{\infty} \frac{1}{2} \left(\frac{2}{\sqrt{\pi}} \kappa r_{\underline{n}ij} \exp(-\kappa^2 r_{\underline{n}ij}^2) + erfc(\kappa r_{\underline{n}ij}) \frac{\underline{r}_{\alpha\underline{n}ij} \underline{r}_{\beta\underline{n}ij}}{r_{\underline{n}ij}^3} + \frac{\pi}{2A} \sum_{\underline{h}}^{\infty} \sum_{i=1}^{N} q_i \sum_{j=1}^{N} q_j B_{\alpha\beta} \Re[\exp(i\underline{h} \cdot \underline{r}_{ij})], \qquad (7)$$

where for
$$h \neq 0$$
,

$$B_{\alpha\beta} = \delta_{\alpha\beta}F(\kappa,\underline{h},r_{zij}) + h_{\alpha}h_{\beta}h^{-2}\{(r_{zij}-h^{-1})\exp(hr_{zij})erfc(h/2\kappa + r_{zij}\kappa) - (r_{zij}+h^{-1})\exp(-hr_{zij})erfc(h/2\kappa - r_{zij}\kappa) - \exp(hr_{zij})\exp(-(h/2\kappa + r_{zij}\kappa)^2)/\kappa\pi^{1/2} - \exp(-hr_{zij})\exp(-(h/2\kappa - r_{zij}\kappa)^2)/\kappa\pi^{1/2}\}$$
(8)

where $\delta_{lphaeta}$ is the Kronecker delta. For, h=0 we have,

$$B_{\alpha\beta} = \delta_{\alpha\beta} F(\kappa, \underline{h} = 0, r_{sij}).$$

(9)

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Shell model Simulations

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David Fincham discussed the calculation of the pressure in the shell model of polarisable ions. In this model ions are represented by a "core" and a "shell", both carrying charges, and connected by a harmonic spring. In the "ideal" shell model the shells have zero mass, and relax instantaneously to zero force positions. In shell-model molecular dynamics using the "adiabatic" method of Mitchell and Fincham (J. Phys.: Condes. Matter 5 (1993) 1031) the shells have a small mass, and their motion is integrated by normal m.d techniques. The ion is therefore treated exactly as if it were a diatomic molecule. However, the shell mass is chosen small enough that the spring frequency remains well above the lattice vibrational frequencies. In these circumstances the core-shell internal degree of freedom does not thermalise and its temperature remains very low. This ensures that the results agree with the ideal model.

Since the internal degree of freedom is not in thermal equilibrium with the other degrees of freedom, it is preferable to approach the pressure calculation from a mechanical rather than a thermodynamic point of view. Such an approach may be based on the virial theorem, which is derived in the textbooks of Hansen and McDonald and of Haile using arguments only from classical mechanics: One can then decide to apply the virial theorem either to the "diatomic molecules" (ions) or to the "atoms" (core and shell). In the "molecule" approach the kinetic term involves only the centre- of-mass (COM) or translational kinetic energy, and the virial term involves COM separations and total molecule-molecule forces. In the "atoms" approach one must include the internal kinetic energy as well as the translational kinetic energy. The virial term includes the virial of the "bonds" as well as the atom-atom intermolecular terms.

The "molecule" and "atom" approaches must agree when ensemble averages are taken. However, a stronger statement can be made. In the ideal (zero shell mass) shell model, the two approaches give identical instantaneous pressures. This is because the shells are always in zero force positions, and then the bond virial is cancelled by the term which converts from the atom-atom to the centre-centre virial. In the adiabatic shell model the two methods give instantaneous pressures which are still equal to an excellent degree of approximation. The details will appear in a forthcoming publication by Fincham, Mackrodt and Mitchell.

Simulation of bilayers

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Mike Allen discussed the calculation of the pressure for a system in which a bilayer of amphiphilic molecules separates two regions of aqueous phase. This had come up in discussions with colleagues at Bristol and elsewhere. Since the number of amphiphiles is fixed, the situation is distinct from the one where a bulk oil layer (for example) separates two regions of aqueous phase. (In both cases we assume full periodic boundary conditions, so really there is just one region of aqueous phase). In the latter case, a change in crosssectional area is associated with a surface free energy term (due to interfacial tension). In fact, it can be calculated from the profiles of the normal and transverse components of the pressure tensor, for a constant-volume simulation. For given numbers of oil and water molecules, a constant pressure simulation may be carried out with the cross-sectional area

fixed and the box length (in the direction normal to the interface) varying. In the case of amphiphiles, there is also a free energy due to the surface, but it is not of the same form, and the surface tension is not well defined. The bilayer is (by definition) microscopically thin, and the pressure tensor profiles are not defined unambiguously on this length scale. The number of amphiphiles per unit cross sectional area must be specified. For fixed values of these parameters, constant pressure simulations allowing the longitudinal box dimension to vary, may be carried out. It is instructive to consider constant-pressure simulations with all three box dimensions varying. For the oil/water case, assuming an isotropic applied 🔆 pressure, the surface free energy term would drive the box towards a long thin shape, so as to minimize the surface area; this could be prevented by applying an anisotropic pressure to oppose the surface energy term, but this would require prior knowledge of the surface tension. In the bilayer case, contant pressure box moves in the transverse direction would change the surface area per amphiphile and the system would stabilize at a certain value of surface area. This seems a reasonable method of equilibrating towards a typical, physically interesting, value for the ratio of surface area per amphiphile, prior to fixing the box area for production runs. As a set any set and set any set any set of set of set of the a second design of the second second

The Isotropy of the Pressure in Anisotropic Systems

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The virial equation gives the pressure tensor, $p_{\alpha\beta}$, in terms of the equilibrium $z_{\alpha\beta}$ ensemble average of the microscopic stress tensor, $\sigma_{\alpha\beta}$. Thus we have

 $p_{\alpha\beta}V = \langle \sigma_{\alpha\beta} \rangle$ $\sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} \right) = \sum_{i=1}^{n} m \overline{\upsilon}_{i\alpha} \overline{\upsilon}_{i\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\alpha} f_{ij,\beta} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} f_{ij,\alpha} f_{ij,\alpha} + \gamma_2 \sum_{i\neq j} \gamma_{ij,\alpha} + \gamma$

where V is the volume of the system, m is the particle mass, \mathbf{v}_i is the velocity of particle i, \mathbf{r}_{ij} is the centre of mass separation between particles i and j and \mathbf{f}_{ij} is the force exerted on particle i by particle j. The Greek subscripts indicate Cartesian tensor components. Eq. (1) presupposes that the system considered is classical and that the forces are pairwise additive.

The pressure tensor is thus an average of a second rank tensor. Let us consider an arbitrary second rank tensor, $A_{\alpha\beta}$, dependent on the molecular configuration. In the isotropic phase, it must be true that

$$\left\langle A_{\alpha\beta}\right\rangle = a\delta_{\alpha\beta}$$

(2)

where n is a scalar constant. Thus it follows that the pressure tensor must also be

isotropic, i.e. assesses which as a start of the sub-section of the sub-section of the sub-

$$p_{\alpha\beta} = p\delta_{\alpha\beta}$$

where p is the normal pressure. The second state is the second state of p and p and p are second state of p are second state of p and p are second state of p

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Now let us consider an anisotropic system, in particular a nematic liquid crystal, where there is a preferred molecular alignment along a particular direction – the director, $\hat{\mathbf{n}}$. Here the average of an arbitrary second rank tensor is not isotropic. In general one has

$$\left\langle A_{\alpha\beta}\right\rangle = a\delta_{\alpha\beta} + b\hat{n}_{\alpha}\hat{n}_{\beta} \tag{4}$$

(3)

with *a* and *b* both being scalar constants. A nematic liquid crystal is a fluid, however, and experimentally one knows it cannot support an external stress. One would thus expect the pressure tensor to be isotropic. The question thus arises as to whether one can show mathematically that there is something special about the stress tensor, so that its average is indeed isotropic and that the constant, *b*, in eq. (4) turns out to be zero. I should point out that there is absolutely no symmetry reason for this property and, indeed, I could make no progress in this matter simply by staring at the virial expression, eq. (1), as it stood.

2. A Proposed Resolution

Let us introduce the Fourier transforms of the microscopic number and momentum densities, n_k and $p_{k,a}$ respectively. These are given by

$$n_{\mathbf{k}} = \sum_{i} \exp(i\mathbf{k} \cdot \mathbf{r}_{i}) \tag{5a}$$

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$$p_{\mathbf{k},\alpha} = \sum_{i} p_{i,\alpha} \exp(i\mathbf{k} \cdot \mathbf{r}_{i})$$

where r_i is the centre of mass of particle i and p_i is its momentum. We have the results that

$$\dot{p}_{\mathbf{k},\alpha} = ik_{\beta}\sigma_{\mathbf{k},\beta\alpha}$$

where the R.H.S. of eq. (7) is exactly the same quantity as appears in eq. (1). Schofield showed that for small k, [1]

$$ik_{\mu} \left(\frac{\partial p_{\alpha\beta}}{\partial \rho}\right)_{\mu} = \frac{\left\langle ik_{\alpha} \sigma_{\mathbf{k}|\alpha\beta} u_{-\mathbf{k}} \right\rangle}{\left\langle n_{\mathbf{k}} u_{-\mathbf{k}} \right\rangle} \tag{8}$$

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where ρ is the average number density of the system and T is the temperature. Eq. (6) and the dot switching properties of stationary correlation functions allows one to rewrite eq. (8) as

$$ik_{\alpha} \left(\frac{\partial p_{\alpha\beta}}{\partial \rho}\right)_{\mu} = -\frac{\left\langle p_{k,\beta} \dot{n}_{-k} \right\rangle}{\left\langle n_{k} n_{-k} \right\rangle} = \frac{ik_{\beta} \left\langle N \right\rangle k_{\beta} T}{\left\langle n_{k} n_{-k} \right\rangle}$$
(9)

where $\langle N \rangle$ is the average number of particles in the system and k_B is Boltzmann's constant. As the low k limit of $\langle n_k n_{-k} \rangle$ does not depend on the direction of **k**, then eq. (9) implies that

(5b)

(6)

$$\left(\frac{\partial p_{\alpha\beta}}{\partial \rho}\right)_{I} = \lim_{k \to 0} \frac{\langle N \rangle k_{B} T}{\langle n_{k} n_{-k} \rangle} \delta_{\alpha\beta}$$
(10)

This is the compressibility equation of state and it shows the density derivative of the pressure tensor to be isotropic. To get the actual pressure tensor we must integrate eq. (10) with respect to density, leaving us with a result of the form

$$p_{\mu\nu} = p\delta_{\mu\nu} + C_{\mu\nu}(T) \tag{11}$$

where the final term is the constant of integration. As the thermodynamic state of a nematic liquid crystal is determined simply by ρ and T, then the constant of integration can only depend on the temperature. As is well known from the virial expansion, however, there exist no density independent terms in any expression for the pressure, so clearly the constant of integration is zero and we have proved that the pressure tensor is isotropic. A rather brief account of this work appears in the appendix of reference [2].

3. Some Final Comments

The argument in the previous section, up to eq. (10) goes through for all systems at equilibrium, solids included. The argument can be generalised to deal with solids under external stresses and strains by making use not only of the zero k limit of n_k but also investigating values of k close to a lattice vector (at least in the case of crystals). Following though this type of approach leads eventually to a disguised expression for Hooke's law. The case of a glass can also be treated but is a little more complicated.

Finally I would like to acknowledge the contribution of Martin Whittle, who first

raised the question with me as to why pressures in anisotropic systems should be isotropic and the contribution of Mike Allen, as it was in the course of collaborative work with him that the solution given above was found.

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DL_POLY: A macromolecular simulation package

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The following is a summary of the DL_POLY presentation given at the recent CCP5 AGM at Keele University, 17 September 1993...

The DL_POLY package is funded by the SERC through the SBCC (Science Board Computing Committee - which has recently changed it's name to the SMCC (Science Materials Computing Committee)). The motivation of the package is to provide a parallel macromolecular simulation package free to the academic community. The reasons for this are many. For example, while there are a number of commercially available (parallel) macromolecular simulation packages, these often have the drawback that they are not free. Moreover, while these packages tend to have very good "front ends" getting to the source code that drives the simulation dynamics can be difficult. Thus in these "black boxes" it can be difficult to know what the package is actually doing to the simulation and modification or extension of the code is not easily achieved. The DLPOLY package is designed to avoid these problems. The source code is freely accessible, extensively documented and highly modular in nature. We wish to avoid the "black box" approach to simulation by providing code that is readily accessible to both verification and modification by users. The package is thus aimed at users who desire intelligent and informed control over their simulations. The package comes as a series of modules that the user "bolts" together for their own particular application. A series of "makefiles" is provided to facilitate this. The package is able to handle a broad range of macro systems - from material science applications (e.g. crystalline and amorphous solids) to simulation of molecules of biological interest (e.g. DNA, enzymes etc) plus a good deal in between. The target machines are Multiple Instruction Multiple Data (MIMD) parallel machines (eg. the Intel iPSC/860 at Daresbury) and single processor workstations. The idea being that users have a code that both works efficiently on a workstation and that will be quite painless to transfer onto parallel supercomputers should they gain access to such facilities. In developing this package beyond a basic capability we are dependent upon the support of the CCP5 community, for example, to supply additional modules for analysis or system generation.

We have adhered to a fairly stringent programming style. All modules are in FOR-TRAN 77 (modules written in C are acceptible provided they are FORTRAN callable). Variables and arrays are passed as arguments through subroutine calls to faciliate the interfacing of modules. Consequently there are no common blocks present in the source code. The modules are also extensively documented, the release I documentation totals about 220 pages.

Features currently available:

Release I is built around two basic strategies. The first is that of "Replicated Data" meaning that all processors have a complete copy of the atomic co-ordinates, velocites and forces but that evaluation of pair-wise interactions, integration of the equations of motion, application of constraints etc are split equally among the available processors. This approach works well for systems of up to at least 20000 particles and on machines with up to 100 or so processors. It has the advantage that the algorithm will run just as readily on a single processor as on a parallel machine, it is relatively straightforward to program, and results in excellent parallelisation efficiences. When the number of processors become very large the algorithm suffers from global communication costs (the requirement that arrays etc are summed globally across all processors), but communication overheads also affect other parallelisation strategies. Replicated data is also more memory intensive that other strategies (e.g. domain decomposition) but we do not consider this to be a serious restriction at present. The second intrinsic feature of the code is that it is atomistic in nature - each site is assigned a mass, charge, coordinated etc and evaluation of the Verlet neighbourhood list is done on the basis of site-site separations At present we do not have the capacity to handle rigid body equations of motion, massless sites and so forth nor to base real space cutoffs on a "molecular group" strategy.

Other features in the package are given below. In each case the required feature is selected by setting an integer variable in the job CONTROL file. As the package is modular in nature additional features are readily added simply by defining new properties for additional values of the integer keys. For example, all evaluations of periodic images take place within one subroutine ("images") and additional periodic boundary conditions can be introduced simply by modifying this single subroutine. Note that all the features that follow are couched in the Replicated data / Atomistic code framework.

- A selection of periodic boundaries (free space, cubic, orthorhombic, parallelopiped, truncated octahedral, rhombodal dodecahedral, two dimension periodicity)
 - A selection of electrostatic methods (three dimensional Ewald sum, Coulombic, truncated and shifted Coulombic, distant dependant dielectric constant)
 - All common atom-atom potentials.
 - Flexible bonds and rigid bonds (SHAKE).
- Valence angle and dihedral angle potentials
- A selection of canonical thermostats (Nosé Hoover and Gaussian constraints) and the non-canonical Berendsen thermostat.
- Single and multiple timestep algorithms
- On-line radial distribution functions and mean squared displacements. The general policy is that analysis routines are intended to be used off-line. This is because the analysis required is usually quite problem specific and so not incorporated into the release package. RDF's and MSDs are however almost univerally required and

it makes sense to calculate them "on-line". They can be turned "on" or "off" by keys in the job CONTROL file. The second construction are stored as a second second second second

· Utility modules to aid in generation of initial configurations. These include setting up lattice structures, creating structures from database files (such as PDB files), and adding thermalised water to a structure.

• A series of utilities to aid in generation of force field files - particularly for polymer and bio-simulations. Utilities for helping generate GROMOS and AMBER force fields are included, as another section of the draw and a section of the section

• Analysis routines: Correlation functions and statistical analysis. These are designed for off-line analysis.

The figure shows the performance of DL POLY as a function of the number of processors in use. The test case is an antifreeze protein emmersed in 1234 SPC waters. Cubic periodic boundary conditions are in use and electrostatic interactions are calculated using the Ewald summation. The plot shows log(average time per step) vs the dimension, d, of the hypercube. The number of processors in use is 2^d and ranges from 2 through to 64 processors. On this plot perfect parallelization would correspond to lines with slope -1. This is what is seen for all subroutines except the reciprocal space summation in the Ewald sum (Ewald1) and for SHAKE. The "perfect parallelisation" is a consequence of the Replicated data strategy as no (or very little) inter-processor communication is required during these parts of the calculation and the work is equally shared among the processors. This is true for tasks such as construction of the Verlet neighbourhood list ("parlst"), and evaluation of real space pair interactions ("Ewald2" and "Srfrce"). However for the subroutines "Ewald1" and "SHAKE" some inter-processor communication is unavoidable and the timing of the program reflects this especially as the number of processors increases. Eventually these algorithms become communication bound, that is, there is no reduction in execution time by using a larger number of processors. The second se

Features in development:

Display modules for use with AVS.

Features for future development:

We hope to begin working soon on algorithms that will facilitate the simulation of "mega-systems" - ie. multi-million particle simulations. In particular this will mean exploiting the "domain decomposition" parallelization strategy and exploring the use of "heirachical multipole" methods for efficient handling of long range (e.g. electrostatic) potentials.

In addition there are several developments that can be added within the Replicated Data strategy, these include:

• Algorithms for rigid bodies (and massless sites).

승규는 전문을 많을 수 있었는 것 같아요.

- Algorithms for constant pressure simulations
- Inclusion of anisotropic site potentials (e.g. Distributed multipoles).

The first two on this list are straightforward to implement and their implementation is dependent on us finding the time to include them in the package. The last item on the list includes some unresolved problems with handling torques on sites contained in a flexible molecular unit. Note that none of these features will be included in DL_POLY release I.

Availability of the code:

Ultimately the package will be available by anonymous ftp from CCP5. However in the intervening 18 months or so from now the package will be available on restricted release within the U.K. only. Those interested in this limited release should initially contact us at Daresbury for more information.

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CCP5 ANNUAL MEETING

LARGE SCALE MOLECULAR SIMULATION

Keele University, 15th - 17th September, 1993

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ORAL PRESENTATIONS

COMPUTER SIMULATIONS OF COMPLEX FLUIDS

B. Smit

Shell Research, B.V. Amsterdam, The Netherlands.

Self assembly of emphilphilic molecules is of importance in a variety of processes ranging from the transport of molecules through cell membranes to the removal of stains in a washing machine. It is shown that computer simulations can be used to study the self-assembly of these surfactant models. Moreover these simulations can be used to study dynamical processes with time scales that span as much as six decades experimentally. These simulations are made possible through the use of efficient algorithms for parallel computers.

Despite the availability of these high performance parallel computers, information on phase equilibria of complex fluids is still very difficult to obtain. In the second part of this lecture it is shown that recent advances in Monte Carlo simulations of complex fluids allows us to determine phase equilibria of complex fluids.

COMPUTATIONAL CHEMISTRY ON WORKSTATION CLUSTERS: PARALLEL PROGRAMMING FOR MOLECULAR DYNAMICS, NEURAL NETWORKS AND GENETICS ALGORITHMS

Dr. Stephen Fleischman

Convex Computer Corporation, 3000 Waterview Parkway, Richardson, Texas 75083, USA

Clusters of RISC workstations provide a very cost effective way to obtain high performance computing. By using fast RISC workstations nodes connected by high speed networks such FDDI, supercomputer level computer performance is possible with the use of course grained, message passing parallelism. The use of workstation cluster computing with three types of computational chemistry applications: molecular dynamics, neural networks and genetics algorithms, will be discussed.

Several molecular dynamics programs have been parallelized and have shown very good improvements in computational speed. We have obtained a 6.0 times acceleration with the program CHARMM on a eight node HP735 cluster using FDDT, for a 14000 atom myoglobin dynamics calculation.

Feed-forward/back-propagation neural networks have been used in to predict protein secondary structure, NMR chemical shifts, for analysis of spectra. This technique is intrinsically parallelizable and three different approaches will be discussed.

A novel 'molecular dynamics-like' algorithm will be presented. Using a leap-frog integrator, the network pattern learning converges much more rapidly than with the more common steepest descent minimization method. A pseudo-temperature thermostat can be applied and simulated annealing performed. The use of this method in protein secondary structure prediction will be described.

Genetics algorithms are stochastic optimizers that can be used for global minimum searching that are also amenable to parallel computing. Their use in conformational searching will be discussed.

COMPLEX FLUIDS AND INTERFACES

M. P. Allen⁽¹⁾, E. de Miguel⁽²⁾ and E. Martini⁽²⁾

⁽¹⁾H.H. Wills Physics Laboratory, Royal Fort, Tyndall Avenue, Bristol, BS8 1TL, U.K.

⁽²⁾Dept. Fisica Atomica Molecular y Nuclear, Univ. de Sevilla, Apartado 1065, Sevilla, Spain

We have carried out simulations of molecular fluids using the Gay-Berne potential, studying the liquid-vapour interface, the structure of the liquid near a rigid wall, and the effects of confinement between parallel walls. In this poster we present density and orientation profiles, discuss the calculation of the interfacial tensions, and the occurrence of layering at the interfaces.

SIMULATION STUDIES OF SMECTIC LIQUID CRYSTALS

Matt Glaser^(1,3), Rainer Malzbender⁽¹⁾, Noel Clark⁽¹⁾ and David Walba⁽²⁾

 (1) Department of Physics, University of Colorado, Boulder, CO, U.S.A.
 (2) Department of Chemistry, University of Colorado, Boulder, CO, U.S.A.
 (3) FOM Institute for Atomic and Molecular Physics, Amsterdam, The Netherlands

Liquid crystalline materials are characterized by an extremely sensitive dependence of bulk properties on molecular structure. We have recently begun a program of realistic (atomic-detail) molecular dynamics Simulation studies of smectic liquid Crystals in an attempt to elucidate structure-property relationships in these materials. We report our initial findings from simulations of bulk samples and freely suspended thin films of several smectic A and smectic C liquid crystals, with an emphasis on understanding the origins of molecular tilt in the smectic C phase:

Work supported by the National Science Foundation Materials Synthesis and Processing Program (DMR-9202312).

A COMPUTER SIMULATION OF THE CLASSIC EXPERIMENT ON OSMOSIS AND OSMOTIC PRESSURE

⁽¹⁾S. Murad and ⁽²⁾J.G. Powles

⁽¹⁾Chemical Engineering Department, University of Illinois at Chicago, Chicago IL 60607 U.S.A. ⁽²⁾Physics Laboratory, University of Kent, Canterbury, Kent, UK.

A novel computer simulation technique for studying fluids in confined geometries has been developed and used to replicate Pfeffer's experiment on osmosis in semipermeable membranes in 1877. Our results confirm the validity of van't Hoff's famous relationship for osmotic pressure over a wide range of concentrations. We believe this is the first theoretical validation of this result for such a wide range of concentrations, where no explicit assumption of ideality is made for the interactions of the solute molecules.

LARGE SCALE MOLECULAR DYNAMICS SIMULATIONS

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Los Alamos National Laboratory and Thinking Machines Corporation

We will review some recently developed Molecular Dynamics MIMD alogirthms using message-passing on the CM-5. These scalable codes attain good speed-up and efficiency for large systems on large numbers of processors. Production runs with dozens of millions of molecules are now possible. We will present performance numbers and discuss some of the applications of these methods in Statistical Mechanics and Materials Science.

MOLECULAR DYNAMICS FREE ENERGY CALCULATION IN 4 DIMENSIONS

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Thomas Beutler and W.F. van Gunsteren

Physical Chemistry, ETH Zentrum, ETH Zuerich, CH-8092 Zurich, Switzerland

A new method for the calculation of free energy differences in molecular dynamics simulation is presented. The main characteristics of the method is, that the physical space is augmented by a further dimension. In physical states, the dynamics along the 4th coordinate is uncoupled from the dynamics described with the original 3 coordinates. In the method presented here, free energy differences are determined using pathways leading over states where the dynamics along all 4 dimensions are coupled. Due to the barrier lowering in 4 dimensions, in many cases an increase of efficiency can be expected. Applications will be given.

MOLECULAR DYNAMICS SIMULATIONS OF DNA TRIPLE-HELICES

C.A. Laughton

CRC Biomolecular Structure Unit, Institute of Cancer Research, Sutton, Surrey, SM2 5NG, U.K.

In view of the current paucity of experimental structural data, the molecular modelling of DNA triple helices plays a particularly important role in helping to understand more clearly their structure and the factors contributing to their stability. We have used molecular modelling, and particularly molecular dynamics; to study both (polypurine).(polypyrimidine).(polypyrimidine) and (polypyrimidine).(polypurine).(polypurine) triplexes. The importance of treating solvation and electrostatic interactions in as accurate a manner as possible is clear, resulting in the need for large scale molecular simulations.

DYNAMIC OF SELENIUM CHAIN MELTS E. Enciso⁽¹⁾, N.G. Almarza⁽¹⁾ and F.J. Bermejo⁽²⁾

⁽¹⁾Dpto. Quimica Fisica I, Facultad de Quimicas, Universidad Complutense, 28040 Madrid, Spain

⁽²⁾Instituto de Estructura de la Materia, CSIC Serrario, 123 Madrid 28006, Spain.

A large scale molecular dynamics (MD) study of linear selenium chain melts is presented. The computed structural and dynamic properties show a good agreement with neutron diffraction experiments. Diffusion and viscosity, transport coefficients are obtained. The single atom or chain motions offer us different spatio-temporary dynamic regimes which for short chains are well described by the Rouse model. The collective dynamics is explained in terms of trapping of the atoms in some spatial regions of the liquid defined by atomic cross-links of the chains. The dependence of those properties with the length of the chain is also studied.

A DATA-PARALLEL MOLECULAR DYNAMICS METHOD FOR LIQUIDS WITH COULOMBIC INTERACTIONS

Fredrik Hedman⁽¹⁾ and Aatto Laaksonen⁽²⁾

⁽¹⁾Parallelldatorcentrum, KTH S-10044 Stockholm, Sweden ⁽²⁾Division of Physical Chemistry, Arrhenius Laboratory, SU S-10692 Stockholm, Sweden

An efficient approach to large-scale data-parallel molecular dynamics for simulations of systems which include Coulombic interactions is presented. Short-range interactions are calculated with a method based on the coarse-grained cell method. In this method the simulation cell is decomposed into equally sized subcells, with the shortest side being larger than the cut-off radius of the short-range interaction. Electrostatic interactions are calculated using a data-parallel version of the Ewald summation method. Calculations of long- and short-range interactions are merged by a suitable choice of the size of the subcells and the Ewald sum parameter.

We avoid a large fraction of the non-productive short-mage and real-space calculations by a geometric sorting procedure based on particle distances to subcell boundaries. Due to particle migration, the contents of the subcells need to be updated. This is done with a method based only on nearest-neighbour communications. Special "null-particles" are introduced, which act as buffers durign periodic updates and allow for a globally uniform alogirthm during the force calculations.

The method, which should be easy to implement on most massively parallel computers of SIMD or MIMD type has been developed on a 8K CM200 using CM Fortran, and so far it has been tested on systems of up to 1 million particles.

MOLECULAR DYNAMICS SIMULATIONS OF CALAMITIC AND DISCOTIC LIQUID CRYSTALS USING A HYBRID GAY-BERNE LUCKHURST ROMANO POTENTIAL

 $M.P.Neal^{(1)}$, $M.D.DE Lucat^{(2)}$ and $C.M.Care^{(3)}$

⁽¹⁾ School of Mathematics and Computing, University of Derby, U.K.
 ⁽²⁾Division of Applied Physics, Sheffield Hallam University, U.K.
 ⁽³⁾Materials Research Institute, Sheffield Hallam University, U.K.

We report a molecular dynamics computer simulation study of a system of particles interacting via an anisotropic potential proposed by Luckhurst and Romano and modified by scaling with part of the well depth formalism employed by Gay-Berne. Parameters are selected to model calamitic mesogens and the systems exhibited a variety of mesophases as the temperature is lowered. The phases are provisionally identified as isotropic, nematic, a highly ordered fluid phase with some smectic features and crystal. Comparison is made with a previous study with the same potential parameterised to model discotic mesogens.

A NEW APPROACH TO MODELLING COMPLEX FLUIDS

userses and the X.F.Yuan, R.C.Ball and S.F.Edwards and a set of the

Cavendish Laboratory, Madingley Road, Cambridge CB3 OHE, U.K.

A new numerical simulation technique for modelling complex fluids, such as polymers, foams, concentrated emulsions and suspensions, has been developed. Using a comoving Voronoi mesh, the method is able to track the details of fluid, e.g. deformation and stream line. The primary results include a johnson-Segalman fluid and a single-integral Doi-Edwards fluid in a simple planar channel, and a Giesekus-Leonov fluid and a Oldroyd-B fluid through a planar 4:1 abrupt contraction at the modestly high Weissenberg number. A extrusion flow is also considered. The simulation methods to deal with foams,; concentrated emulsions and suspensions are presented.

MOBILITY OF WATER AND CATIONS AT SILICATE SURFACES

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Department of Earth Sciences, Parks Road, Oxford, OX1 3PR, U.K.

Molecular Dynamics computer simulations have been used to study the microscopic processes of fluid transport and dynamics in layered silicates (clay minerals). The model system is an idealized Otay-montmorillonite with both MG and Na counterions. The calculations yield quantitative water diffusion rates which agree well with experimental neutron-scattering results. Their temperature dependence indicates the operation of more than one activated diffusion process; at room temperature the activation energy is 11.1+/- kJ/mol. Cation diffusion is much slower than that of water and is insigificant on the simulation timescale.

NANOSECOND MD SIMULATIONS ON DNA OLIGONUCLEOTIDES IN WATER

D.L. Beveridge

Department of Chemistry and Molecular Biophysics Program, Wesleyan University, Middletown, CT 06459, U.S.A.

A series of MD simulations on DNA dodecamers including solvent explicitly have been carried out on the nanosecond time scale. Various options for including counterions or emulating counterion condensation have been investigated. The simulations are based on the GROMOS force field augmented with a hydrogen bond potential for Watson-Crick base pairing. Special considerations on the problem of truncating potentials will be described. Analysis of the convergence characteristics, conformational and helicoidal parameters and major and minor groove width are included. The results are compared in detail with experimental data from x-ray crystallography and NMR spectroscopy. The sequences considered are duplex d(CGCGAATTCGCG) and d(CGCAAAAAACGG).

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SIMULATIONS OF MATERIALS: THE NEXT BEST THING

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School of Physics, Georgia Institute of Technology, Atlanta, Georgia 30332, U.S.A.

Knowledge of the properties of materials on the atomic scale is of key importance for developing a fundamental understanding of materials systems, as well as for the elucidation and solution of a large number of technological problems. Computer-based simulations open new avenues for investigation of materials processes with high-resolution in space and time. Such simulations, coupled with high resolution experimental microscopies, guide formulations of atomic and molecular materials design principles for technological uses, and provide "virtual reality" images of the microscopic nature of the materials world.

In this lecture the methodology and practice of modern classical and quantum computer simulations of various materials systems and phenomena, will be discussed. Examples include: structure, energetics, and dynamics of electron localization in small water droplets; fission dynamics of clusters; atomistic description of friction and lubrication; phase transitions and dynamics of segregatrion in adsorbed complex molecular liquid films;and collision dynamics of clusters impinging onto solid and liquid surfaces. The presentation will include computer generated animations of the atomistic dynamical evolution of materials systems.

PATH ENERGY MINIMIZATION: A NEW METHOD FOR THE SIMULATION OF CONFORMATIONAL REARRANGEMENTS IN LARGE MOLECULAR SYSTEMS.

Oliver S. Smart

Department of Crystallography, Birkbeck College, University of London, Malet Street, London WCIE 7HX, England.

Conformational transitions play an important role in biological processes, e.g. substrate binding, ion transport and allosteric transformations in haemoglobin. Existing simulation methods for the generation of reaction paths can be applied for conformational changes in small molecules but are not suitable for large scale transitions in macromolecules. A new method for the generation of a reaction path linking two known conformers of a molecule is presented. The path energy minimization technique is based on optimizing a function which approximates the peak potential energy of a series of positions between the minima. The method is applied to simulate a substantial conformational transition of the ion-channel forming peptide gramicidin A and is shown to have a large radius of convergence but to be computationally costly in the present implementation. Methods for obtaining the overall optimal route once the transition state is identified will be discussed.

POSTER PRESENTATIONS

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MOLECULAR DYNAMICS SIMULATIONS OF OLIGONUCLEOTIDES O⁶ METHYLGUANOSINE

Keith A. Parker, Leonor Cruzeiro-Hanson and Julia M. Goodfellow

Department of Crystallography, Birkbeck College, Malet Street, London, WCLE 7HX, U.K.

A variety of compounds such as N-methyl-N-nitrosourea and N-ethyl-N-nitrosourea are known to cause alkylation of the O^6 atom in guanine residues. This alkylation has been shown to induce the misincorporation of thymine opposite the O^6 -methyl guanine (meG) in the template strand. On replication this leads to adenine pairing with this thymine and hence a modified guanine has been effectively transformed into an adenine. The formation of O^6 -alkylguanine is a fundamental event which, if not repaired by the enzyme O^6 -alkylguanine-DNA-alkyltransferase, may lead to a carcinogenic lesion.

Alkylation of the O^6 atom of guanine causes a loss of the N1 proton which affects subsequent base pairing arrangements. The conformation of the O^6 -methyl group with respect to the complementary base may also have an effect on base-pairing. If the distal conformation (i.e. cis to N1) is adopted disruption of base-pairing is considerably more than if the methyl group is in the proximal conformation (trans to N1).

We have undertaken a number of molecular dynamics simulations on oligonucleotides containing the methylated base O⁶-methylgauanine in order to determine the conformation and flexibility of such sequences. The total time course of these simulations being 1000 ps with the last 120ps being used for the analysis. The conformations of a normal Watson-Crick and a G-T mismatch sequence, generated by a similar procedure, are entirely consistent with the available experimental data. The sequence containing, methylguanine base paired with thymine (meG-T) is iso-structural with the normal sequence, irrespective of the conformation of the methyl group, but with only two hydrogen bonds between the bases. In contrast, the conformation of the sequence containing methylguanine base-paired with cytosine (meG-C) depends on the orientation of the methyl group and shows clear differences to normal Watson-Crick hydrogen bonding and would more likely be recognised by repair enzymes.

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COMPUTATIONAL SORPTION STUDIES OF ALKANES IN ZEOLITES

Michael G.B. Drew and Paul M. Hobbs

Chemistry Department, University of Reading, Whiteknights, Reading, Berkshire, RG6 2AD, U.K.

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Alkaline sorption in a pentasil zeolite has been studied through molecular simulations. A series of alkanes, including methane, propane, n-butane, iso-butane and three hexane isomers, were studied in silicalite. Statistical mechanical principles have been employed to predict sorption equilibria at low occupancy. Henry's constants and isosteric heats of sorption were calculated, using the CERIUS software package from Molecular Simulations, through the evaluation of configurational integrals with a Monte Carlo integration scheme. A range of Lennard-Jones parameters for carbon, hydrogen, silicon and oxygen were used. The effects of using united atoms in the alkane and of removing the silicon atoms from the zeolite were estimated. An optimised set of parameters were obtained to fit with experimental data for n-hexane and then used subsequently with other alkanes. The results were in good agreement with other literature experimental values⁽¹⁾. This work has been funded by Molecular Simulations, cambridge and B.P., Sunbury.

(1) J.R. Hufton, R.P. Danner, AIChE Journal, 1993, Vol. 39, No. 6, pp. 954-961.

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DYNAMICS WITH THE SHELL-MODEL

Dr. P.J.D. Lindan of the test state of the test

Laboratoire des Solides Irradies, Ecole Polytechnique, 91128 Palaiseau Cedex, France.

Potentials for ionic materials are among the best classical models currently available, giving very realistic descriptions of many physical properties. The key feature in providing this realism has been found to be the inclusion of ion polarisability, most often via the shell model. Until recently though, the dynamical properties of such models, and their comparison with experiment, have received little attention due to the computational workload involved in dealing with the extra degrees of freedom.

We discuss here recent progress in the dynamical simulation of ionic materials using shell-model potentials. This includes the approaches which have successfully been developed to deal with the central problem, which is the requirement that the system obeys the Born-Oppenheimer principle with respect to the polarisation. The results of extensive simulations of U02, using the best potentials available, and comparison with neutron-scattering and other experimental data show the feasability of shell-model MD, and also shed new light on the capabilities of the potentials.

ORIENTATIONAL PHASE BEHAVIOUR IN AN INTERFACIAL MONOLAYER OF DISCOTICS. A MONTE CARLO STUDY

2018년 8월 2019년 18월 2019년 18월 21일 문화

Richard Edwards and Jim Henderson

School of Chemistry, University of Leeds, Leeds, LS2 9JT, U.K.

Results of an isothermal-isobaric Monte Carlo simulation study of a monlayer of disc-shaped molecules are presented, with special reference to the orientational phase behaviour. In our model, molecules with disc-shaped repulsive cores are constructed from seven equally-sized hard spheres of diameter σ , bonded at contact such that their centres all lie in a plane. The six outer spheres of each molecule are attracted to the substrate by a square-well field of range $\sigma/2$ and depth ε_{ω} . In addition, the centres of each molecule attract each other through a spherically-symmetric square-well of range 3σ and depth ε . To ensure the monolayer condition, the discs are constrained such that at least one of the six outer spheres is in contact with the wall field at any given time. Each simulation involves three fixed thermodynamic fields: temperature $T^* = kT/\varepsilon$, surface field strength $h^*1 = \varepsilon_{\omega}/\varepsilon$, and surface pressure $p^* = p\sigma^2/\varepsilon$, conjugate to the area of surface coverage, A. At high pressures, in the presence of a weak surface field, condensed-liquid phases are observed in which the molecules adopt vertical orientations with respect to the surface and formations of chain-like structures are observed in pseudo-smeetic domains. At low pressures, in the presence of a strong surface field, expanded-liquid phases become increasingly favoured and the molecules adopt a horizontal configuration.

A MODULATED BULK AS A FUZZY BOUNDARY FOR THE SIMULATION OF LONG-RANGED INHOMOGENEOUS SYSTEMS

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Juan Carlos Gil Montoro and J.L.F. Abascal

Depto Quimica Fisica, Fac. Ciencias Quimicas, Universidad Complutense, 28040 Madrid, Spain.

A new method for simulating infinite dilution inhomogeneous systems with long-ranged electrostatic interactions which make no use of artificial perturbating boundaries is presented. The inhomogeneous system extends its effect through a cell of the appropriate symmetry which is in turn immersed in a box with bulk solution. The boundary between the inhomogeneous and homogeneous regions can be freely crossed by the moving particles. The particles interact with the surrounding bulk through a discrete particle-particle modulated Coulomb potential while the missing tail is recovered as a mean field contribution computed in a self-consistent way. The bulk particles undergo usual periodic boundary conditions.

The modulated bulk as fuzzy boundary method have been checked with MC simulations of the cylindrical model of polyelectrolytes using soft continuous potentials. Comparison with previous simulations of the same model is done.

SCANNING KERR MICROSCOPY STUDIES OF ARTIFICIAL MAGNETIC STRUCTURES

U. Ebels, E. Gu, A. Adeyeye, J.A.C. Bland

We describe a Laser-Scanning-Kerr-Microscope (LSKM), designed to combine studies of the macroscopic magnetic properties, i.e. spatially averaged, with studies of the microscopic magnetic properties e.g. magnetic domain structures and local hysteresis loops with aspatial resolution of approximately 1 m. In both cases the sample can be rotated relative to the applied field in order to distinguish between hard and easy axes. In the focused geometry the insertion of an aperture in the incoming beam path allows the in-plane magnetisation components to be resolved and thus making a vector analysis of the magnetisation in a domain possible.

The feasibility of the LSKM system is demonstrated by measurements on a polycrystalline 115A. Co/GaAs (110) film and on polycrystallne micron sized magnetic grating structures (1050 A Fe/GaAs).

One and two dimensional scans of the 115 A Co/GaAs film show magnetic domain contrast with domain sizes of the order of 5 to 10 μ m, which is consistent with domain images of this sample taken by Lorentz Microscopy. Further the lorentz Microscopy domain images can be understood in terms of the strong uniaxial anisotropy found in local hysteresis loop measurements.

In the Fe/GaAs grating structures the effect of a strong shape anisotropy due to the wires is

AN MD STUDY OF CHAIN CONFIGURATIONS IN N-ALKANE LIQUIDS

Dr. D. Brown

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We present precise measurements of the configurational properties of n-alkane-like liquids with 4, 5, 8, 20, 50 and 100 methylene groups. Quantities measured include the distributions of square radii of gyration, square end-to-end distances and proportion of conformiers. To achieve high precision a Fujitsu AP1000 massively parallel processing machine with up to 1024 processors has been used in both a "cloning" and domain decomposition mode and the efficient implementation of a constraints algorithm within the latter framework will be discussed. The results are compared with those obtained for the Flory model of alkane chains in which only correlation between nearest-neighbour torsion angles are considered; the latter were obtained by Morite Carlo sampling of isolated chains using the pivot algorithm. Discrepancies between the two sets of data are discussed in terms of solvent and end effects.

MOLECULAR DYNAMICS OF DNA DODECAMERS INCLUDING ALKYLATED BASES

L. Cruzeiro-Hansson, K. Parker and J.M. Goodfellow

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N-nitroso compounds alkylate DNA and are potent carcinogens in most species. An understanding of the mechanism by which N-nitroso compounds induce mutations and cancer involves the characterization, on a molecular scale, of the effects that methylation has on DNA. Using the AMBER force field, we apply MD methods to investigate the structure and dynamics of four dodecamers which have similar sequences, i.e. they differ only at basepairs four and nine, which are either thymine or 0⁴-methylthymine, basepaired with either thymine's usual counterpart adenine, or with guanine. Very long simulations (i.e. 1000 ps) are made to ensure equilibration and an extensive analysis is performed on the thermodynamic ensemble of conformations. A comparison of the simulations with the available experimental data indicates that the conformations obtained in the simulation are reasonable representations of the structure of the dodecamers in solution. The effect of alkylation on the base pairing of adjacent bases, on the helical parameters as derived from CURVES, such as xdisp, roll, rise, twist, and propeller twist and on the backbone conformation including sugar puckering is analysed. We find that the dodecamer in which the modified thymine is paired with guanine is more isostructural to the regular DNA duplex than the dodecamer in which the modified thymine is paired with adenine. The biological implications of this and other findings are analysed.

MC SIMULATION OF FIRST ORDER PHASE TRANSITIONS IN VO2

B. Slater and M.G.B. Drew

University of Reading, Department of Chemistry, Whiteknights, Reading RG62AD

VO₂ undergoes a first-order phase transition at 340 K, from a monoclinic distorted rutile phase to tetragonal. Using Monte Carlo techniques previously applied to modelling nucleation processes¹, the free-energy barrier separating the phases can be sampled. The intermolecular potentials used were generated using the program PARAM² by minimising the first derivatives of the lattice energy with respect to the lattice constants. Relaxation of each structure produced ensembles with RMS values of les than 0.1A, with respect to the crystal structure. The Monte Carlo simulations using 768 atoms show that there is a small free-energy barrier separating the distorted structure from the more thermodynamically stable phase. The transition is achieved easily, reproducing the crystal structure well. The reverse path is less favourable and more severe conditions are required to facilitate the transition.

¹ J.S. van Duijneveldt and D. Frenkel, J. Chem. Phys., 96 (6) 1992.
 ² V. Padayatchy, Ph.D. Thesis, University of Reading.

CATION/ANION-WATER INTERACTIONS IN ALUMINOSILICATES AND MOLECULAR MODELLING OF HYDRATION IN CA-ZEOLITE A

Paul Barnes⁽¹⁾ and Antony Richards⁽²⁾

 (1) Birkbeck College, Malet Street, London, U.K.
 (2) Molecular Simulations, St. John's Innovation Centre, Cowley Road Cambridge, CB4 4WS, U.K.

Aluminosilicates span a wide range of technologically important materials from cements to zeolites. Great effort has understandably, been expended in the study of zeolite action using both experimental and modelling/simulation techniques, but whereas anhydrous systems have been extensively investigated the important role of hydration has been somewhat neglected.

The aim of this work is to redress the balance by (a) deriving an effective tool-kit of interatomic potentials for modelling the role of water in the synthesis and function of several basic aluminoscilicate materials of industrial importance and (b) to use these potentials in a Monte Carlo simulation to study the mechanism of hydration in an experimentally well characterised system.

The former investigation is an extension of the previously published work of Aloisi et al who derived a method for calculating interatomic potentials, novel in the way the surrounding local ion/counter-ion environment is accounted for, and in how the repulsion component is extracted and the parameters fitted to a Buckingham type potential.

The simulations used the Molecular Simulations CERIUS molecular modelling software into which the new set of potential parameters for the water-cage interaction had been incorporated. The results were in agreement with various published work and illustrated the most favourable positions for the water molecules to reside as the system becomes increasingly hydrated. The cations present were effectively seen to block access to the bega cage through the 6-membered rings. From these simulations a mechanism for hydration/dehydration is postulated.

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SIMULATION OF CHIRAL SOLVENT EFFECTS

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Experimental measurement and molecular dynamics simulations have been used to study solvent effects on the circular dichroism (CD) of the n-pi* transition. The systems studied have been bromocamphor in the achiral solvents carbon tetrachloride and n-hexane. It was found that the solvent may make significant contribution to the CD intensity; this arises because the bromocamphor can induce a solvation structure that is chiral even when the solvent molecules themselves are achiral. The magnitude of the solvent effect is found to depend strongly upon the nature of the solvent. This has implications for enhancing the enantiomeric selectivity of chiral synthesis.

COMPUTER SIMULATION OF POLYMER PHASE SEPARATION

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The very early stage of phase separation of a blend of two different polymers induced by a change of temperature was investigated through computer simulation of a polymeric system. The system is a model system which represents a blend of two different polymers in liquid state. The polymers are modeled as real chains. The computer simulation was done by a method of molecular dynamics simulations (MDS). The MDS was used to simulate a system which is in equilibrium with it's environment which maintains certain fixed temperature and pressure. At first, two polymers are in a mixed state at a temperature at which they are miscible. At a given time, the temperature drops to a lower temperature at which the polymers become immiscible and the system starts a phase separation. The computer simulation shows that at least there are two different stages of phase separation during the first few hundred pico seconds. In the first stage which lasts about a few tens of pico seconds, small phase separated domains are formed rapidly. The driving force for this rapid process is the initial sharp drop of total potential energy induced by separation of energetically unfavourable two different species. The formation of small domains in the first stage of phase separation is determined by the density fluctuations of each species in the miscible state. The process of phase separation in the second stage appears to be a lot slower than the first one. The driving force of phase separation is the reduction of total potential energy of the system, and the total potential energy drops very rapidly in the first stage and then it decreases slowly in the second stage. In the second stage, the size of domains remain almost the same and the boundaries between domains are becoming sharper. The maximum time spanned by MDS in this work is about a few hundred picoseconds. Therefore, this work is limited to the dynamics of phase separation during the first few hundred picoseconds. It is conceivable that there are more distinct stages of phase separation after the first two stages shown in this computer simulation. One of the most important aspects of dynamic of polymers is the effect of entanglement among chains. It is shown that this effect is fully implemented in the computer simulations.

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STUDIES OF LIQUID CRYSTALS BY CONSTRAINED MOLECULAR DYNAMICS

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We have developed a method of conducting molecular dynamics simulations of liquid crystal phases with constraints applied to the director. This approach allows one to conveniently calculate transport coefficients and elastic constants in the director-based frame. It will also permit the calculation of orientation-dependent free energies and allow control of the director orientation relative to interfaces in large-scale simulations of liquid crystals. We have carried out trial simulations using this method for the Gay-Berne potential, and report our results in this poster.

ENERGETIC FULLERENE INTERACTIONS WITH SILICON AND GRAPHITE CRYSTAL SURFACES

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The interaction of C60 molecules with silicon crystal surfaces is modelled using molecular dynamics. The results are compared to similar interactions with graphite surfaces. It is found that the molecule rarely reflects intact from the Si surface. When reflection does occur it is always at near grazing incidence with impact energies less than 300eV. At normal incidence and similar energies the molecule remains intact, but becomes embedded in the surface layers of the Si lattice. Grazing incidence ($-75^{\circ}-80^{\circ}$ to the surface normal) at energies of a few hundred. eV results in the fullerene molecule becoming trapped in the surface binding potential. The molecule can roll across the surface for up to one revolution before coming to rest. At energies of greater than ~500eV, at grazing incidence; the molecule breaks up on impact with the majority. of the constituent atoms reflected. Normal incidence with impact energies in excess of I keV leads to disintegration of the fullerene molecule and sputtering from the crystal, with the ejection of atoms and larger SixCy molecules. This is especially evident, at energies greater than 4 keV where high energy deposition near the impact point creates a crater surrounded by a hot disordered region from which Si atoms can be thermally ejected for times up to the order of 1ps. At normal incidence on graphite it is found that the C60 molecule is reflected intact at energies up to about 25OeV and a depression wave spreads radially from the point of impact across the graphite surface preceded by hypersonic fronts which transmit small amounts of energy. At energies of 1keV and 6keV the molecule implodes as it enters the crystal creating a region of dense amorphous carbon beneath the surface. Very little sputtering occurs at normal incidence at energies of up to 6keV. At 6keV and at an incidence angle of 60° to the normal, the molecule breaks up on impact and some sputtering is observed. At 15keV the sputtering yield increases and the surface ruptures in the central region where carbon clusters and chains are ejected. Outside this region the bonds remain intact but surface begins to separate from the second layer with a raised travelling wave propagating from the impact point.

MONTE CARLO SIMULATION OF NON-IONIC SURFACTANTS IN WATER

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Monte Carlo simulation studies of interfacial water structure and chain conformation in non-ionic surfactant bilayers were used in an attempt to explain the nature of hydration forces.

Simulations of a single attached polyoxyethylene surfactant chain and polyoxyethylene bilayers at a fixed bilayer separation have been performed at various temperatures. The observed gauche/trans ratio increase and stronger chain adsorption with increasing temperature is explained by increasing chain repulsion. Hence, increasing hydration forces with temperature is proposed.

COMPUTER SIMULATION AND THEORY FOR WARD-SPHERE CHAIN MODELS OF LIQUID CRYSTALS

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Isothermal-isobaric (NpT) Monte Carlo simulations are used to determine the thermodynamic and structural properties of linear chains of tangent hard spheres over a wide range of densities. Chains of m=2 to 7 spheres have been examined to date. The simulations are performed in rectangular boxes starting from hep initial configurations; in certain cases the rectnagular box is allowed to vary in shape. The low-density liquid phases are compressed to higher densities. Simulations are also started from perfectly aligned high-density solids which are melted to low-density phases. Reptation moves are performed to speed up equilibration. The types of phase transitions obtained by expanding the solid and compressing the liquid are examined. In the case of the dimer (m=2), a plastic solid phase is formed when the system is compressed. The systems with m=3 and 5 form glassy states when the liquid is compressed, whilst the aligned solids melt directly to the isotropic liquid. In contrast to previous suggestions for the system m=4, liquid crystalline phases are not observed. Preliminary results show that the hexamer (m=6) exhibits an isotropic-liquid crystal phase transition. A study of the effect of molecular flexibility on ordered phases will be undertaken to determine the maximum amount of flexiblity that will sustain these phases. We have also used a simple Onsager theory to examine the phase transitions exhibited by systems of hard spherocylinders defined by a length-to-breadth ratio of L/D. Two major problems with the usual Onsager approach are the speed of convergence of the solutions and the poor agreement with simulation for systems with small or intermediate aspect ratios. We present a simple extension of the theory with an improved repulsive term. The free energy function is examined using a Monte Carlo annealing method which is rapidly convergent and easy to generalise. Comparisons are made with the results of simulation,

COMPUTATIONAL STUDIES OF HYDROCARBON DIFFUSION IN ZEOLITES

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We report results of MD simulations of n-butane and n-hexane adsorbed in zelite Silicalite at different loadings and temperatures. Our production runs are necessarily long (1000 ps) due to the slow diffusion observed in these systems. We simulate the adsorbate molecules by means of the Ryckaert-Bellemans model for alkanes, and, at present, we consider a rigid zeolite framework. Our results show that the conformational distributions of the adsorbates and their transport properties are substantially affected byt he presence of the zeolite framework. Diffusion is seen to take place by means of a hopping mechanism. The calculated diffusion coefficients are in good agreement with experimental values, but the use of a rigid framework model seems to prevent the thermalization of adsorbate molecules at low loadings, and unrealisticially large hopping distances are observed in such cases.

MONTE CARLO SIMULATION OF LIQUID CRYSTAL PHASE TRANSITIONS

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We have implemented special biased sampling and windowing techniques in Monte Carlo simulations to obtain details of the order parameter distribution function and free energy close to the isotropic-nematic phase transition. These techniques are capable of locating the position of the transition, and determining its order, with greater accuracy than was possible before. We have tested these methods on various simple hard particle models, using extremely long runs, and report the results in this poster.

SIMULATIONS OF SILICATE GLASSES

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Realistic MD simulations have been performed on the silicate glass Na₂ Si₂ O₅ over a wide range of temperatures. The simulations have generated a structure that strongly resembles that deduced from experiment. An investigation of the conductivity of the material has revealed the low diffusion of the sodium ions within the silicate framework and produced an Arrhenius activation energy close to that seen experimentally. Studies are continuing to establish the details of the diffusion processa the microscopic level.

MD SIMULATION OF IONIC SYSTEMS WITH A LONG RANGE INTERACTION APPROXIMATION INCLUDING IONIC STRENGTH EFFECTS

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In MD simulation various treatments of the long-range electrostatic forces have been used. We propose a long-range force expression which treats the medium outside the cut-off radius in terms of the linearized Poisson-Boltzmann (PB) equation. The expression is based on the analytical solution of the PB problem for a sphere containing an arbitrary charge distribution surrounded by a dielectric continuum with a ionic strength. Molecular dynamics simulations for a system of 1M NaCl solution in water have been performed. The method is compared with the results obtained by application of the Ewald summation technique.

INHIBITION OF THE CRYSTAL GROWTH OF GAS HYDRATES

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Solid gas hydrates form in gas piplines so blocking and reducing the efficiency of gas flow. This study uses Monte Carlo and Molecular Mechanics methods to look at a growth inhibitor, polyvinylpyrrolidone (PVP), and the mechanism by which units of the polymer adsorb to the hydrate surface. Adsorption sites are identified using the monomer analogue N-ethylpyrrolidone (N-EtPy).

UNFOLDING OF LYSOZYME DRIVEN BY A RADIUS OF GYRATION DEVIVED POTENTIAL

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Unfolding of a protein can be monitored by the increase in its radius of gyration. It was therefore tempting to ask if a penalty function involving the latter in an MD simulation could be used to drive unfolding and if yes, following which pathway.

Various trial potentials have been applied to lysozyme as a test system and appeared to give quite different results than simulated thermal unfolding at 500K.

DIRECT FREE ENERGY CALCULATIONS FOR CLATHRATE HYDRATES

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In this work we present a method of calculating the water contribution to the free energy of water clathrates using a modified quasiharmonic/local harmonic model. The method has been used to calculate the free energy of the empty hydrate over a range of temperatures and pressures and the results compared with calculated and experimental values for several ice structures.

The effect of cavity occupancy on the stability of clathrate hydrates has been studied to examine the extent to which the lattice relaxes in the presence of guest molecules.

PROPERTIES OF LIQUID CRYSTAL PHASES FORMED FROM SEMI-FLEXIBLE CHAIN MOLECULES.

Mark R. Wilson

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Molecular dynamics simulations have been carried out on systems of semi-flexible chain molecules composed of hard spheres. The simulations use the rattling spheres model of Chapela et al ^[1]. In this model hard sphere sites are are linked together by means of narrow potential wells with infinite barriers. Each chain consists of seven spheres with each sphere bonded to its neighbour(s) with additional hard wall constraints ensuring that non-adjacent spheres do not overlap ^[2].



Four model systems have been studied with each system differing from the others through a different set of constraints^[3]. These differing constraints ensure that each model system exhibits a different amount of flexibility.

At high density nematic and smectic-A liquid crystal phases are seen for these systems. Results are presented describing the properties of the bulk fluids together with single-particle molecular properties within these phases.

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[2] M. R. Wilson, and M. P. Allen (1993). A computer simulation study of liquid crystal formation in a semi-flexible system of linked hard spheres. Molec. Phys., in press.

[3]M. R. Wilson (1993). Molecular dynamics simulation of semi-flexible mesogens. Molec. Phys., in press.

¹ And set 0.5 sets on the experimental product of a management of the test factor of the set XT model (species) 5 bits fitted bases of the set of the method bases are not set species and the sets.